Consistent Modeling of Discrete and Continuous Mechanics

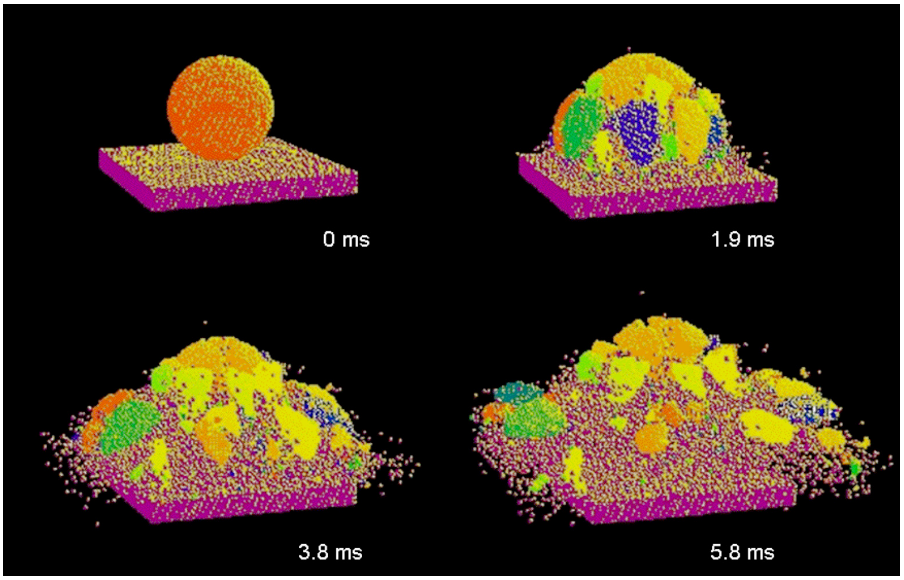

Figure 1: Because the peridynamic theory can treat any number of mutually interacting dynamic fractures, it provides a natural way to model fragmentation. This computer calculation reproduces fragmentation due to the impact of a brittle sphere against a rigid wall.

Peridynamics could lead to higher fidelity in physical simulations and provide a new pathway to the goal of multiscale modeling of materials

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Many researchers have attempted to couple the standard differential equations of continuum mechanics with discrete models for atomic and molecular systems. There have also been many efforts to couple models for crack growth with models for continuum mechanics. What these efforts have in common is that they try to connect mathematical systems that are fundamentally dissimilar from each other: one set of equations for the continuous model, and another for the discrete. This leads to the need for complex and sometimes problematic coupling techniques.

Sandia researchers have asked the question: What would happen if, instead of coupling dissimilar mathematical systems, the same physical phenomena could be modeled within a single, consistent set of equations? These same equations would be applicable everywhere in a body, regardless of whether it is treated as a set of discrete particles or as a continuum, and regardless of whether cracks or localizations form. The hypothesis is that such a mathematically consistent model could lead to higher fidelity in physical simulations and could provide a new pathway to the goal of multiscale modeling of materials.

The method involves developing a new theory of continuum mechanics called the *peridynamic* model. This theory treats discrete particles, fracture surfaces, and continuous bodies all with exactly the same equations. It accomplishes this by using integral equations rather than partial differential equations. Mechanically, the integral equations represent direct interactions between points in a body within a predefined distance of each other, called the horizon. The peridynamic model does not use stress and strain; these are concepts that are important in the standard theory, but which hinder application to discrete systems. Instead, the Sandia model characterizes the internal forces within a body in terms of force densities between points in a body. The model therefore has a natural similarity to molecular dynamics. Figures 1 and 2 illustrate some of the advantages of the peridynamics model.

A number of significant accomplishments have emerged from this effort: (1) In the limit as the horizon approaches zero, it was proved that the peridynamic equations converge to the partial differential equations of the standard theory. In this sense, the standard theory is a subset of the peridynamic theory. (2) It was shown that a set of discrete classical particles, such as atoms interacting through a multibody potential, can be modeled exactly as a peridynamic body. (3) The notion that the integral equations of peridynamics can be obtained from statistical physics was also demonstrated. (4) A peridynamic energy equation that contains a more general notion of work conjugacy than in the classic theory was derived. (5) Sandia implemented the peridynamic model within LAMMPS, its widely used molecular dynamics software.

The expectation is that these recent advances will enable Sandia to use the peridynamic theory as a mathematically consistent framework in which to coarse-grain atomistics into a continuum model.

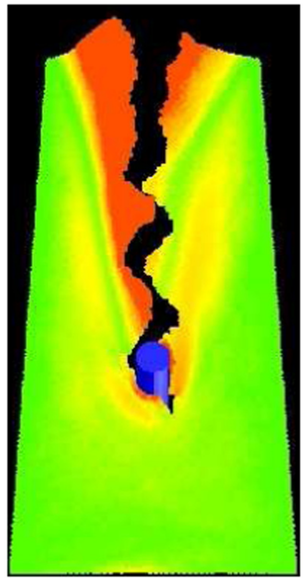

Figure 2: Mathematically consistent treatment of discontinuities reveals subtleties in the mechanics of fracture. Here, a peridynamic simulation reproduces the instability that results in a wavy crack trajectory in a membrane pulled past a rigid cylinder.